

Glutaric acid, nonyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C27H36O5/c1-2-3-4-5-6-7-11-20-30-26(28)18-13-19-27(29)31-22-23-14-12-17
InchiKey:	MDUYUZJINNZRGU-UHFFFAOYSA-N
Formula:	C27H36O5
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	440.57

Physical Properties

Property code	Value	Unit	Source
gf	-181.19	kJ/mol	Joback Method
hf	-760.84	kJ/mol	Joback Method
hfus	60.14	kJ/mol	Joback Method
hvap	101.63	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.986		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinqol	3390.00		NIST Webbook
tb	1050.50	K	Joback Method
tc	1286.11	K	Joback Method
tf	625.96	K	Joback Method
vc	1.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.77	J/molxK	1050.50	Joback Method
cpg	1276.39	J/molxK	1246.84	Joback Method
cpg	1269.54	J/molxK	1207.57	Joback Method
cpg	1261.11	J/molxK	1168.31	Joback Method
cpg	1251.04	J/molxK	1129.04	Joback Method
cpg	1239.28	J/molxK	1089.77	Joback Method
cpg	1281.71	J/molxK	1286.11	Joback Method
dvisc	0.0000149	Paxs	1050.50	Joback Method
dvisc	0.0000193	Paxs	979.74	Joback Method

dvisc	0.0000259	Paxs	908.99	Joback Method
dvisc	0.0000366	Paxs	838.23	Joback Method
dvisc	0.0000552	Paxs	767.47	Joback Method
dvisc	0.0000904	Paxs	696.72	Joback Method
dvisc	0.0001654	Paxs	625.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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